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## **Peer-review statement**

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# Germany-wide time series of interpolated

# phenological observations of main crop types

## between 1993 and 2021

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## 15 ABSTRACT

The data descriptor represents a Germany-wide and spatio-temporally consistent  $1 \times 1 \text{ km}^2$  analysis-ready time series of interpolated days of the year (DOYs). The data set covers 56 entry dates of phenological development stages of 9 main crop types for the period between 1993 and 2021. The derivation of the 1624 records is based on phenological observations are related by Corman Material Service (MND) and the DUASE model which combines the concert of graving degree

<sup>16</sup> provided by German Meteorological Service (DWD) and the PHASE model, which combines the concept of growing degree days (GDD) with a geostatistical interpolation procedure. Each data set is characterized by the global accuracy metrics *R*<sup>2</sup> and *RMSE*. The data are stored as datacubes in the rasdaman Array DBMS which also serves to offer it via APIs based on the open OGC standards. A main application of the resulting data set is the extraction of phenological windows for any available year and user-defined region. This information is relevant for agricultural applications such as weather or biodiversity index derivation, crop-type classification, soil erosion, crop yield modeling or integrated pest management.

## 17 Background & Summary

<sup>18</sup> Plant phenological stages represent annual and periodically recurring plant physiological events or plant developmental stages<sup>1</sup>.

<sup>19</sup> Monitoring of phenological events has a long tradition and is carried out in different regions worldwide<sup>2,3</sup>. The German

20 Meteorological Service (DWD) has maintained a nationwide monitoring program for decades, with about 1200 volunteer

observers reporting the entry dates of about 160 phenological growth stages ( $\equiv$  phases) in a standardized form<sup>4</sup> based on the

internationally accepted BBCH scale (Table 1)<sup>5</sup>. The direct inter- and intra-annual use of the observations for the entire German territory is associated with several challenges:

• Before the reunification of the two German states, two separate observation programs were maintained. Since 1992, the

two German phenological observation programs have been unified. This means that there are no observations for eastern

<sup>26</sup> Germany before 1992 (Figure 1a and b). In addition, due to changes in the observation program, not all classes have

been continuously observed. This concerns, for example, phases 22 and 23 of winter wheat, whose monitoring was

discontinued in 1992, or oat, where the observation program was interrupted between 1992 and 2014 (Figure 1c and

d). While continuous observations between 1992 and today are available for winter wheat, this is not the case for oat.

- <sup>30</sup> Therefore, the oat phases are not part of the data set presented here.
- The phenological observation network of the DWD belongs to the oldest European volunteered geographical information (VGI) programs<sup>4</sup>. Although the observations of the annual reporters go through a quality control process<sup>4</sup>, phenological VGI are often associated with inconsistencies in terms of environmental conditions, geographic location, or timing of observations<sup>7,8</sup>.
- For the practical use of the observations, the distances between the actual observation site and the respective study area

Phase name	PHASE ID (DWD)	BBCH ID
Greenup	1	-
Beginning of flowering	5	61
Full flowering	6	65
End of flowering	7	69
Beginning of sowing	10	0
Emergence	12	10
Closed stand	13	35
4 <sup>th</sup> leaf unfolded	14	14
Beginning of shooting/stem elongation	15/67	31
Beginning of leaf formation	16	12
Beginning of bud formation	17	50
Beginning of heading/tassel emergence	18/66	51
Beginning of milk ripening	19	75
Early dough ripening	20	83
Beginning of yellow ripening	21	87
Beginning of full ripening	22	-
Harvest	24	-
1 <sup>st</sup> cut for hay	25	-
1 <sup>st</sup> cut for silage	26	_
Tip of tassel emergence	65	53

Table 1. Names and identifiers of DWD phenological phases<sup>6</sup> and corresponding BBCH equivalents<sup>5</sup>.

must be taken into account<sup>9</sup>. This is complicated by the fact that the observations are characterized by both spatial variability and spatio-temporal gaps<sup>10</sup>.

To improve the spatio-temporal availability of phenological information, the PHASE model was introduced<sup>12</sup>. The model couples the Growing Degree Days (GDD) concept with a geostatistical interpolation procedure. Based on the PHASE model, the data descriptor represents a Germany-wide and spatio-temporally consistent  $1 \times 1 \text{ km}^2$  analysis-ready time series (ARTS) of interpolated Day(s) of the Year (DOY) covering the potential entry date of phenological development stages (phases) of 9 main crop types for the period between 1993 and 2021. In total, there are 56 phases or three to nine different phases depending on the specific crop type.

A main application of the resulting data set is the extraction of phenological windows for any available year and user-defined region<sup>13</sup>. This information is relevant for applications such as agricultural weather or biodiversity index derivation, crop-type classification, soil erosion, crop yield modeling or integrated pest management<sup>10, 14–21</sup>.

The dataset is published and citeable via Digital Object Identifier (DOI)<sup>22</sup> following the FAIR principles to improve the findability, accessibility, interoperability, and reuse of digital (geo)data<sup>23,24</sup>. Furthermore, the data publication is linked to a Web Coverage Service (WCS) enabling a standardized web-based retrieval and analysis of spatio-temporal geospatial information<sup>25,26</sup> (see Data Records section). Finally, the used algorithms are documented in a software repository to make the life cycle of the data sets reproducible<sup>27</sup> (see Code Availability section).

## 52 Methods

## 53 PHASE model

The PHASE model represents a collection of **R** scripts<sup>28</sup>. Figure 2 shows the corresponding process chain of individual functions, which can be divided into the three groups (a) input data preparation, (b) temperature summation and (c) interpolation. Using the example of the phenological phase *heading* (phase ID = 18) of winter wheat (plant ID = 202) for the vegetation period 1999/2000, the most important steps of the process chain are described in the following sections. Compared to the

<sup>58</sup> original PHASE model<sup>12</sup>, some modifications have been made in the current variant:

GDDs are defined as the sum of daily mean temperature above a crop-specific base temperature<sup>29,30</sup>. The PHASE model calculates GDDs for each year, phase and location. The resulting phase- and year-specific distribution is subjected to a statistical filtering operation, which aims at the detection of observation inconsistencies. In this way, the model fit can be

 $_{62}$  improved significantly, but the number of samples is thereby reduced considerably<sup>12</sup>. This fact is significant because the



**Figure 1.** Spatial coverage of observations using the example of the winter wheat phase *heading* (Phase 18) for 1992 (a) and 2000 (b) as well as yearly temporal observation coverage of phenological phases for winter wheat (c) and oat (d; Table 1).



**Figure 2.** PHASE model process chain: relations between functions for the derivation of year- and plant-specific phenological phases<sup>11</sup> (P – Phases, F – standard deviation interval filter, nF – no Filter).

number of observations has drastically reduced over the years. Figure 3 illustrates the situation using the example of
 phenological observations for winter wheat, which have decreased between 1993 and 2021 to one quarter of the 1993
 sample number. Hence, the modification aims at a trade-off between sample number and model fit (see Methods section).

The original PHASE version uses a *Regression Kriging* variant<sup>31</sup> as the interpolation method, with a digital elevation model (DEM) serving as an additional explanatory variable. However, as the number of observations has decreased by both the applied filtering operation as well as by fewer reports over the years, the number of samples is often too small to

derive reliable variograms. As a consequence, a spline algorithm was applied for the actual interpolation of phase-specific

<sup>70</sup> DOYs, which allows spatial forecasting models with a smaller number of samples<sup>32</sup> (see Methods section).

## 71 Input data preparation

72 After activating all necessary packages (function fLoadAndInstall), the procedure starts with the download of all crop-

- r3 specific phenological observations (function fDownloadPhenObs). Then, the downloaded observations are imported
- 74 (function fImportPhenObs) and coupled with phenological stations (function fPhaseStation), which results in a point
- vector dataset of observed phase- and year-specific Germany-wide events (Figure 1). Each file contains station-specific start
- <sup>76</sup> DOYs (column DOY\_start), at which the crop-specific vegetation period begins (Table 2). The start DOY for summer crops can
- be set by user (default value e.g., DOY = 1). For winter crops, the start DOYs correspond to the DOYs of a user-defined phase
- <sup>78</sup> of the previous year. Outliers are removed using the *interquartile range* (IQR) criterion<sup>33</sup>. In Table 2, start DOYs for winter
- <sup>79</sup> wheat in the year 2000 are shown corresponding to the DOYs of phase *beginning of sowing* (Phase ID = 10) in 1999.



Figure 3. Relationships between unfiltered observation sample number (SN) and year for selected winter wheat phases.

The function fLoadTemp imports an interpolated temperature data set for a given vegetation period. The Germany-wide data set is provided by the DWD<sup>34</sup>. For this application, data of each single year are stored in csv format, which is related to a polygon vector dataset representing a Germany-wide weather grid of  $1 \times 1$  km cell size.

For summer crops, the year-specific temperatures are incorporated. For winter crops, the temperatures of the previous year are also included, starting with the minimum Germany-wide observed DOY of the starting phase defined in the function fPhaseStation. In Table 3, an excerpt of an interpolated temperature data set is listed for the vegetation period of winter wheat in the year 2000. The very first DOY of the starting phase *beginning of sowing* (phase ID = 10) was observed on 19 August 1999 (*DOY* = 231), which results in the DOY difference 231 - 365 = -134 and the corresponding temperatures.

## 88 Temperature summation

For a given growing season and phase, the function fTeffSum couples the phenological observations (Table 2) and the daily mean temperatures (T; Table 3). While a vegetation period of summer crops only considers the year of interest, a vegetation period of winter crops starts in the previous year on the DOYs of sowing. According to the equation (1), the plant-specific base temperatures ( $T_B$ ) are subtracted during temperature summation, negative temperatures are deleted, and the remaining temperature values are weighted by a daylength factor (DL). For each phase- and year-specific station, the effective temperatures ( $TS^{eff}$ ) are then accumulated (Table 4). Figure 4 displays a  $TS^{eff}$  density plot for the phenological observations of the winter

<sup>95</sup> wheat phase *heading* in the year 2000.

$$TS^{eff} = \sum_{i=DOY_{start}}^{DOY_{obs}} \left( (T - T_B) \times \frac{DL_i}{24} \right)$$
(1)

The function fDoyCrit filters the phase- and year-specific distribution of effective temperature sums  $(TS^{eff})$  in a two-stage procedure:

(1) Quantiles (Q) with user-defined probabilities p of effective temperature sums ( $TS^{eff}$ ) are calculated according to Equation

(2). In Figure 4, the 0.5 quantile and the quantile value range for the probabilities variants  $p \in [0.3, 0.7]$  are shown.

$$TS^{crit} = Q_p(TS^{eff}) \tag{2}$$

STATION	Ð	X	Y	GRID_ID	ΟΓ	YEAR	PLANT	PHASE	DATE	QF	DOY	DOY_start
10725	268938	3396415	5273501	33965273	10	2000	202	18	20000511	1	131	291
10723	268976	3410415	5279501	34105279	10	2000	202	18	20000516	1	136	281
10768	269201	3426415	5280501	34265280	10	2000	202	18	20000608	1	159	275
10802	268105	3456415	5286501	34565286	10	2000	202	18	20000610	1	161	300
10700	268439	3505415	5288501	35055288	10	2000	202	18	20000528	1	148	295
10786	268538	3523415	5290501	35235290	10	2000	202	18	20000602	1	153	289

**Table 2.** Excerpt of an attribute table of year- and phase-specific phenological stations on example of the winter wheat phase *heading* (phase ID = 18) in the year 2000 (STATION – ID of a phenological observation station, ID – object ID, X/Y – coordinates, GRID\_ID – raster cell ID related to a Germany-wide weather grid, QL – DWD quality level, YEAR – year of observation, PHASE – phase ID, PLANT – crop ID, DATE – date of a beginning phenological phase, QF – DWD quality flag, DOY – day of the year of a beginning phenological phase, DWD\_start – day of the year on, which the crop-specific vegetation period begins).

GRD_D	T-134	T-133	T-132	T-131	T-130	T-129	T-128	T-127	T-126	T-125	T-124	
32805658	152	157	143	136	165	203	250	204	186	180	183	
32805661	153	158	144	137	166	204	250	205	186	181	183	
32815657	153	157	144	137	165	203	250	204	186	181	183	
32815658	152	157	143	136	165	203	250	204	186	180	183	
32815659	152	157	144	137	165	203	250	204	186	181	183	
32815660	153	157	144	137	165	203	250	205	186	181	183	

**Table 3.** Excerpt of an interpolated temperature data set [ $^{\circ}C \times 10$ ] for the vegetation period of winter wheat for the year 2000 (GRID\_ID – raster cell ID related to a Germany-wide weather grid, T[1:365]: daily temperatures [ $^{\circ}C \times 10$ ] of the year of harvest, T[-X:-1] (only for winter crops): daily temperatures [ $^{\circ}C \times 10$ ] of the year of sowing (-X=DOY-365)).

GRID_ID	TON	LAT	STATION	ID	YEAR	PLANT	PHASE	DATE	DOY	DOY_start	T_SUMS
33965273	7,6311	47,5980	10725	1	2000	202	18	20000511	131	-75	2409
34105279	7,8160	47,6540	10723	2	2000	202	18	20000516	136	-85	2580
34265280	8,0288	47,6650	10768	3	2000	202	18	20000608	159	-91	2545
34565286	8,4277	47,7216	10802	4	2000	202	18	20000610	161	-66	4050
35055288	9,0810	47,7410	10700	5	2000	202	18	20000528	148	-71	3208
35235290	9,3212	47,7586	10786	6	2000	202	18	20000602	153	-77	3534

**Table 4.** Excerpt of an attribute table of station- and phase-specific temperature sums (TS=T\_SUMS) on example of the winter wheat phase *heading* in the year 2000 (GRID\_ID – raster cell ID related to a Germany-wide weather grid, LON/LAT – Longitude/Latitude, STATION – ID of a phenological observation station, YEAR – year of observation, PHASE – phase ID, PLANT – crop ID, DATE – date of a beginning phenological phase, DOY – day of the year of a beginning phenological phase, DOY\_start – starting DOY, from which temperature sums are calculated, T\_SUMS – phase- and station-specific temperature sums).



**Figure 4.**  $TS^{eff}$  density plot of phenological observations for the winter wheat phase *heading* in the year 2000, corresponding quantiles with different probabilities  $(Q_{0,3-0,7})$  as well as single ( $\sigma$ ) and double standard derivations  $(2(\sigma_{0,5}))$  for  $Q_{0,5}$ .

(2) The resulting critical effective temperature sums  $(TS^{crit})$  are used to determine the station- and phase-specific DOY  $(DOY^{P})$ 100 when the condition  $TS^{eff} > TS^{crit}$  is fulfilled. 101

(3) The remaining  $TS^{eff}$  distribution is statistically filtered using standard deviation variants resulting from multiplying the 102 standard deviation ( $\sigma$ ) and a user-defined factor (*STD*). Figure 4 shows the positions of the first ( $\sigma_{0.5}$ ) and second standard 103 deviation (STD =  $2 \Rightarrow 2(\sigma_{0.5})$ ) for the 0.5 quantile variant ( $Q_{0.5}$ ).

104

#### Interpolation and accuracy asessment 105

For each filtering variant,  $DOY^{P}$  and observed DOY values ( $DOY^{obs}$ ) are compared by calculating the Pearson correlation 106 coefficient  $(COR)^{35}$ , Root Mean Squared Error  $(RMSE)^{36}$ , and Mean Absolute Error  $(MAE)^{37}$ . By applying the function 107 fFilterAssessment, the optimal filtered observation variant ( $O^{opt}$ ) results from the maximum value of the product of 108 observation sample number (SN) and COR value. Optionally, the MAE value can also be taken into account (Eq. (3)). Table 5 109 contains the accuracy metrics and assessment result for all filtering variants of the winter wheat phase *heading* in the year 2000. 110

$$O^{opt} = \frac{SN \times COR}{(MAE)} \tag{3}$$

The most optimal variant is extracted by the function fOptShp, which corresponds in Table 5 to the 0.40 quantile ( $Q_{0.40}$ ) 111 with a standard deviation factor of STD = 1.5. The final interpolation of the resulting point data set is performed by applying 112 a regression kriging or thin plate spline algorithm<sup>38,39</sup>, respectively, using the winter wheat phase heading in 2000 as an 113 example (function fPhaseInterpolation). Optionally, local accuracy metrics can be derived for each interpolation 114 result, allowing characterization of the local prediction uncertainty of each grid cell<sup>10</sup>.<sup>10</sup>. Here, the interpolation algorithms are 115 associated with the local accuracy metrics Kriging Standard Variance (KSV) and Spline Standard Error (SSE), both of which 116 represent the spatial standard error of estimation<sup>39,40</sup>. 117

Figure 5 visualizes both interpolation variants as well as the corresponding local accuracy metrics. Finally, external global 118 validation is performed in addition to the local accuracy assessment to provide an "indication of the limits of the predictions"<sup>41</sup> 119 (see Technical Validation section). 120

#### **BonaRes repository** 121

The BonaRes Repository ("Soil as a sustainable resource for the bioeconomy") is a domain specific repository tailored to 122 and basically open for soil and agricultural research data, but also for related domains, e.g. hydrological data or weather data 123 typically in tabular (csv, xlsx) or in geodata formats (FeatureClass, KML, shapefile). The repository is designed as a Spatial 124 Data Infrastructure (SDI), since the majority of data that is published originates from the landscape context and is therefore 125 spatial data. Through this SDI, all data are managed and made available for reuse via download and Web Map Service (WMS) 126 based on open and internationally adopted standards. The underlying concept of Research Data Management (RDM) follows 127

the FAIR data principles for improving the findability, accessibility, interoperability and reusability of research data and is in 128

Q	RMSE	MAE	SN	COR	YEAR	STD	PLANT	PHASE	OPT
0.3	4.11	3.51	584	0.85	2000	1	202	18	494.84
0.35	3.99	3.39	589	0.85	2000	1	202	18	502.5
0.4	3.94	3.34	595	0.86	2000	1	202	18	509.13
0.45	4.05	3.38	602	0.85	2000	1	202	18	510.28
0.5	3.97	3.33	589	0.86	2000	1	202	18	503.78
0.55	4.14	3.5	589	0.84	2000	1	202	18	495.96
0.6	4.04	3.44	558	0.85	2000	1	202	18	476.61
0.65	4.17	3.57	543	0.85	2000	1	202	18	461.01
0.7	4.34	3.76	518	0.84	2000	1	202	18	434.65
0.3	5.48	4.63	736	0.74	2000	1.5	202	18	546.01
0.35	5.37	4.51	742	0.74	2000	1.5	202	18	551.22
0.4	5.37	4.49	749	0.74	2000	1.5	202	18	553.85
0.45	5.35	4.44	745	0.74	2000	1.5	202	18	552.78
0.5	5.31	4.42	735	0.75	2000	1.5	202	18	549.64
0.55	5.45	4.56	728	0.74	2000	1.5	202	18	537.79
0.6	5.46	4.6	711	0.75	2000	1.5	202	18	531.12
0.65	5.64	4.8	703	0.74	2000	1.5	202	18	522.15
0.7	5.9	5.09	691	0.73	2000	1.5	202	18	507.15
0.3	6.9	5.73	857	0.61	2000	2	202	18	518.68
0.35	6.77	5.58	861	0.61	2000	2	202	18	521.57
0.4	6.75	5.55	867	0.6	2000	2	202	18	521.25
0.45	6.88	5.62	877	0.59	2000	2	202	18	515.64
0.5	6.97	5.72	879	0.59	2000	2	202	18	515.91
0.55	7.14	5.9	879	0.58	2000	2	202	18	512.07
0.6	7.24	6.01	869	0.58	2000	2	202	18	506.45
0.65	7.29	6.12	851	0.6	2000	2	202	18	508.18
0.7	7.44	6.34	833	0.62	2000	2	202	18	512.5
0.3	8.02	6.52	925	0.51	2000	2.5	202	18	474.83
0.35	7.96	6.43	935	0.49	2000	2.5	202	18	462.67
0.4	7.91	6.38	940	0.49	2000	2.5	202	18	458.5
0.45	7.89	6.36	943	0.48	2000	2.5	202	18	457.31
0.5	7.98	6.45	945	0.48	2000	2.5	202	18	454.27
0.55	8.18	6.66	948	0.47	2000	2.5	202	18	447.24
0.6	8.34	6.84	946	0.47	2000	2.5	202	18	445.24
0.65	8.62	7.13	945	0.47	2000	2.5	202	18	439.93
0.7	8.87	7.43	936	0.47	2000	2.5	202	18	440.54
0.3	8.66	6.95	956	0.45	2000	3	202	18	433.22
0.35	8.49	6.79	960	0.45	2000	3	202	18	427.41
0.4	8.35	6.67	961	0.44	2000	3	202	18	426.99
0.45	8.36	6.67	965	0.44	2000	3	202	18	422.2
0.5	8.45	6.76	968	0.43	2000	3	202	18	415.84
0.55	8.61	6.96	970	0.42	2000	3	202	18	411.93
0.6	8.87	7.2	973	0.41	2000	3	202	18	402.22
0.65	9.08	7.45	970	0.42	2000	3	202	18	403.09
0.7	9.47	7.86	970	0.41	2000	3	202	18	401.62

**Table 5.** Accuracy metrics and assessment results for variants of quantiles and standard deviation filters on example of the winter wheat phase *heading* in the year 2000 (MAE – Mean Absolute Error, MSE – Mean Squared Error, COR – Pearson correlation coefficient. RMSE – Root Mean Squared Error, PLANT – crop ID, PHASE – phase ID, SN – observation sample number, STD – standard derivation factor, YEAR – year of observation, OPT – result of  $COR \times SN$ ).



**Figure 5.** Interpolated DOYs based on *Regression Kriging* and *Thin Plate Spline* (a, c) as well as local accuracy metrics *Kriging Standard Variance* (KSV) and *TPS Standard Error* (SSE) (b, d) for the winter wheat phase *heading* in the year 2000.

	Crop ID							
Phase ID	201	202	203	204	205	208	215	252/253
1	•							
5			•		•		•	
6			•					
7								
10		•	•	•	•	•	•	•
12		•	•	•	•	•	•	•
13								•
14					•			
15		•	•	•		•		
17					•			
18		•	•	•				
19		•				•	•	
20							•	
21		•	•	•		•	•	
22					•			
24		•	•	•	•	•	•	•
25	•							
26	•							
65							•	
66						•		
67					•		•	

**Table 6.** Interpolated Germany-wide phenological phases (see Table 1). 201 – permanent grassland | 202 – winter wheat | 203 - winter rye | 204 - winter barley | 205 - winter rape | 208 - summer oat | 215 - maize | 252/253 - fodder/sugar beet.

line with good scientific practice<sup>23</sup>. It is complemented by a comprehensive description with standardized metadata and DOI 129 assignment<sup>42</sup>. 130

The metadata schema combines all elements of DataCite<sup>43</sup> and INSPIRE<sup>44</sup>, supplemented by detailed attribute metadata that 131 facilitate scientific reuse. Metadata is captured in a user-friendly manner and entered via an online metadata editor, including 132 thesauri (FAO: AGROVOC<sup>45</sup>, EEA: GEMET<sup>46</sup>), licenses (Creative Commons<sup>47</sup>: Attribution 4.0 International (CC BY 4.0)), 133 lineage elements, and data access points (SDI with OGC services such as spatial search and WMS for visualization). 134

The download formats provided in the BonaRes repository (GDB, TXT, CSV, XLSX) are oriented towards the needs of 135 the target group and can be extended upon request (e.g. GeoJSON, KML, GML, GPX). Likewise, the currently offered target 136 coordinate systems (EPSG: 25833, 31467, 31468, 4326) can be extended. 137

Data steward services include in-person support, metadata review, and tools for the entire workflow: Data submission, 138 metadata description, and publication. Due to the broad diversity of soil and agricultural data, customized RDM strategies have 139 been developed to improve data quality and make them easily citable. 140

The BonaRes approach to foster the reuse of published data in the agricultural domain is such that data are compiled into 141 highly aggregated datasets that are useful for reuse. In addition, there is the opportunity to compile datasets into data collections 142 (AGROVOC). Data collections consist of a parent dataset, which contains e.g. the geodata, and several child datasets. All 143 datasets are semantically linked via metadata. In addition, it is possible to represent genuine relations (primary; foreign key) by 144 means of the data model. The parent dataset is the gateway to the data collections and acts as a landing page for the DOI. For 145 reuse and thus citation in scientific journals, this has the advantage of being able to cite various datasets with one DOI. Data 146 collections are arbitrarily expandable. When a download request is submitted, all datasets subordinate to the DOI are initially 147 provided, but can be selected. 148

#### Data Records 149

152

#### Repository data records 150

The PHASE data set is available for the entire area of Germany, covering three to nine phenological phases depending on the 151 crop type (Table 6) and 29 years (1993–2021), resulting in 1624 records. The entire dataset is made available through the

BonaRes repository<sup>48</sup> and contains the following files: 153

- The current crop-specific (PLANT) and year-specific (YEAR) Germany-wide interpolation products are stored as csv files with the naming convention [PLANT]\_[YEAR].csv. Each file contains all year- and phase-specific DOYs (Table 6) and can be coupled to a Germany-wide weather grid via the column GRID\_ID, which corresponds to DWD reference units<sup>49</sup> with a geometric resolution of 1 × 1 km<sup>2</sup>. The weather grid can be downloaded from the PhaseR Github repository<sup>11</sup>.
- Each phase- and year-specific interpolation result is characterized by global accuracy metrics. All crop-specific metrics are summarized in a file with the naming convention VAM\_[PLANT].csv. Table 7 shows the accuracy metrics for the interpolated optimal phenological observation variants for winter wheat phase *heading* for the years 1993 to 2021.
- In addition to the interpolation results and accuracy metrics, the Germany-wide temperature input data are provided
- with the naming convention tmit\_[YEAR].csv. The files do not include a header and contain year-specific gridded temperatures (columns 2-366). Data sets are provided by DWD<sup>50</sup> and can be coupled with DWD reference units<sup>49</sup> with a

geometric resolution of  $1 \times 1 \text{ km}^2$  (column  $1 \equiv \text{GRID}_\text{ID}$ ) of the file [PLANT]\_[YEAR]. csv).

## **Coverages and Web Coverage (Processing) Services**

<sup>167</sup> While the BonaRes repository ensures data availability according to FAIR criteria<sup>42</sup>, web services enables direct ARTS access<sup>25</sup>.

For this purpose, data sets are imported into the PHASE Data Cube (see Usage Notes section). There, the data sets are managed

locally and made available via the Open Geospatial Consortium (OGC) standard WCS<sup>51</sup>. We briefly introduce the coverage
 data and service model.

In ISO, OGC, and INSPIRE the concept of coverages is used to denote "fields" (as in physics) in general, and specifically serve to model multi-dimensional raster data in an encoding-independent manner; both regular and irregular spatio-temporal grids are supported. The central standard is the OGC Coverage Implementation Schema (CIS) which is identical to ISO 19123-2. A coverage data structure consists of four main components (1) the domain (Where are these data located in space and time?), (2) the range (the data values), (3) the range type (What is the structure of the range values and their meaning?) and (4) metadata (any additional information the coverage should carry along). Such coverages can be encoded in the common formate, such as GaoTHEE NETCODE or ISON

- 177 formats, such as GeoTIFF, NETCDF, or JSON.
- Based on the coverage definition above, the WCS standard is defined. Unlike a WMS<sup>52</sup>, which derives map images suitable for human consumption, a WCS allows extraction of spatio-temporal subsets – possibly processed on server side – as the
- original data, which can be interpreted, analyzed, and rendered using any programming language, browser, or geographic
- <sup>181</sup> information system (GIS). The WCS of the PHASE Data Cube is documented in an OpenAPI specification<sup>53</sup>. An example of a
- WCS request extracting from winter wheat, together with the resulting entry dates of phenological stages, is shown in code example 1.

The associated metadata are also standardized and stored as part of the coverage object. This metadata record can be extended with any additional information<sup>54</sup> such as, in an INSPIRE setup, with INSPIRE-compliant metadata<sup>55</sup>. In the WCS code example 2, the metadata of the PHASE Data Cube are queried for winter wheat. The output snippet shows global accuracy measures as they are calculated and stored for all interpolations results (see Technical Validation section, Table 7).

- One of the components of the modular WCS suite is the Web Coverage Processing Service (WCPS)<sup>56,57</sup>, a geo datacube analytics language. It allows for server-side filtering, processing and fusion in a high-level, language-independent way. In our work, we heavily use WCPS as it gives high flexibility and is compact to use.
- The rasdaman Array DBMS is both the OGC WCS reference implementation and INSPIRE WCS Good Practice. In this study, rasdaman is used to manage, server, and analyze all the datacubes (see Usage Note section).

**Code example 1.** WCS query for DOYs of all beginning phenological phases of winter wheat (see Table 6) as csv format for the year 2000 (coverage name: "PHASE\_202\_Winterweizen") and a location near Braunschweig (Germany).

1	https://datacube.julius-kuehn.de/flf/ows?&SERVICE=WCS&VERSION=2.0.1&REQUEST=GetCoverage&
	COVERAGEID=PHASE_202_Winterweizen&SUBSET=ansi("2000-01-01")&SUBSET=E(597930)&SUBSET=N
	(5795243)&FORMAT=text/csv
2	
3	Output: "112.5206 142.4212 172.3821 198.0325 218.6161 275.6248 290.5179"

## **Technical Validation**

<sup>194</sup> While the actual interpolation is performed using all filtered observations (see Methods section), the external validation is

based on a random division into a training and a test data set of 75 % and 25 %, respectively, considering the target parameter

Code example 2. WCS query to recieve metadata for winter wheat phases (coverage name: "PHASE\_202\_Winterweizen").

1	<pre>https://datacube.julius-kuehn.de/flf/ows?&amp;SERVICE=WCS&amp;VERSION=2.0.1&amp;REQUEST=DescribeCoverage     &amp;COVERAGEID=PHASE_202_Winterweizen</pre>
2	
3	Output XML snipped:
4	
5	<record></record>
6	<plant>202</plant>
7	<phase>18</phase>
8	<year>2000</year>
9	<0N>747 0N
10	<mse>26.1050033362502</mse>
11	<mae>4.00605421643839</mae>
12	<rmse>5.10930556301443</rmse>
13	<r2>0.394334005817017</r2>
14	
15	

distribution. The similarity of the two distributions is tested by applying the nonparametric *Kolmogorov Smirnov* goodness-of-fit (KS) test<sup>58</sup>.

<sup>198</sup> Model building is based on the training data set. The test data set is used for validation<sup>59</sup> providing the metrics  $MAE^{37}$ ,

<sup>199</sup> Mean Squared Error  $(MSE)^{60}$ ,  $RMSE^{36}$  and  $R^{261}$ . Table 7 shows the global accuracy metrics for the winter wheat phase <sup>200</sup> *heading* for the years 1993 to 2021.

Figure 6 summarizes the phase-specific accuracy metrics  $R^2$  and RMSE for all interpolation results. In addition, interpolation results based on unfiltered phenological observations were produced (see Figure 2) to illustrate the impact of the filtering and optimization approach on modeling accuracy. Accordingly, the  $R^2$  values of the early phases 10 and 12 are comparable for both categories. Starting with phase 15, the  $R^2$  values of the filtered variants are significantly higher than those of the unfiltered variants. For the *RMSE* values, this is true for all phenological phases. Furthermore, it can be observed that the accuracy values improve with increasing vegetation development, which is related to the diminishing influence of the human factor and the

 $_{207}$  increasing dominance of the temperature sum influence, respectively<sup>12</sup>.

## 208 Usage Notes

As a government research institution, the Julius Kühn Institute (JKI) operates a decentralized, cloud-integrated SDI to perform 209 Big Data analyses of multi-hierarchical geospatial data time series<sup>62</sup>. The JKI SDI consists of three main components that 210 are interoperably connected via standardized interfaces. The main components are the CODE-DE cloud platform for German 211 authorities, which provides direct access to satellite imagery data and processing capabilities, and local JKI (geo)databases or 212 storing vector, raster and metadata. The JKI Data Cube uses the rasdaman Array DBMS, and "gives access to multi-dimensional 213 coverages via WMS for visualization, WCS for data extraction, reformatting, and download, and WCPS for safe server-side 214 analytics"<sup>63</sup> (see Data Records section). The JKI Data Cube is composed of individual thematic cubes that can differ in 215 terms of their spatial and temporal resolution and extent (Figure 7). In addition to the PHASE data cube with phase- and 216 year-specific entry dates (DOY<sup>P</sup>), three other Germany-wide Cubes were used for the usage notes. The DWD\_TEMP\_MAX 217 and DWD\_Niederschlag data cubes are characterized by a geometric resolution of  $1 \times 1$  km<sup>2</sup>, result from interpolated DWD 218 station measurements, and contain daily maximum temperatures  $(T^{d,max})$  and daily precipitation totals  $(P^{d,sum})$ , respectively, for 219 the period from 1961 to the present. The S2 GermanyGrid JKI data cube provides 10 cloud-masked atmospherically corrected 220 spectral bands (Blue, Green, Red, RedEdge1, RedEdge2, RedEdge3, NIR 10 m, NIR 20 m, SWIR1, SWIR2) of the Sentinel-2 221 sensor for the entire area of Germany and the period from 2015 to present. While the S2\_GermanyGrid\_JKI data cubes are 222 stored on the CODE-DE server in Frankfurt am Main, the other data cubes are located at the local JKI SDI in Braunschweig. 223

## <sup>224</sup> WCS-based coupling of phenological, spectral information and weather data

A Jupyter notebook was created to query three different data cubes and obtain a common data set for a single winter wheat plot in Lower Saxony (Germany) in  $2020^{64}$ . In addition to the open PHASE data, multispectral Sentinel-2 imagery and precipitation data are also requested via WCS (Figure 7). The soil-adjusted vegetation index (*SAV1*)<sup>65</sup> is calculated from the Sentinel-2 data to provide information on canopy development throughout the growing season. Finally, a joint plot of all requested data is created (Figure 8).

PLANT	PHASE	YEAR	ON	MSE	MAE	RMSE	R2
202	18	2021	326	14.6	3.09	3.82	0.38
202	18	2020	317	26.49	3.78	5.15	0.34
202	18	2019	342	21.85	3.74	4.67	0.41
202	18	2018	351	24.75	3.77	4.97	0.14
202	18	2017	411	14.93	3.18	3.86	0.46
202	18	2016	361	11.43	2.71	3.38	0.40
202	18	2015	355	26.41	4.02	5.14	0.39
202	18	2014	425	23.4	3.94	4.84	0.30
202	18	2013	500	22.35	3.44	4.73	0.48
202	18	2012	423	16.84	3.14	4.1	0.45
202	18	2011	516	17.3	3.38	4.16	0.57
202	18	2010	512	21.37	3.58	4.62	0.31
202	18	2009	567	16.68	3.24	4.08	0.39
202	18	2008	516	18.89	3.31	4.35	0.28
202	18	2007	451	24.09	3.90	4.91	0.36
202	18	2006	609	15.72	3.08	3.96	0.61
202	18	2005	625	23.87	3.73	4.89	0.47
202	18	2004	634	22.58	3.68	4.75	0.53
202	18	2003	634	14.05	3.04	3.75	0.46
202	18	2002	646	27.86	4.12	5.28	0.31
202	18	2001	563	31.08	4.34	5.57	0.32
202	18	2000	747	26.11	4.01	5.11	0.39
202	18	1999	851	19.58	3.52	4.42	0.36
202	18	1998	782	14.41	2.82	3.8	0.34
202	18	1997	972	21.53	3.59	4.64	0.38
202	18	1996	988	15.92	3.09	3.99	0.30
202	18	1995	991	32.01	4.39	5.66	0.44
202	18	1994	1083	28.57	4.14	5.34	0.37
202	18	1993	1025	20.82	3.56	4.56	0.36

**Table 7.** Global accuracy metrics of the interpolated optimal phenological observation variant for the winter wheat phase *heading* for the years 1993 to 2021 (PLANT — crop ID, PHASE — phase ID, MAE – Mean Absolute Error, Mean Standard Error, RMSE – Root Mean Square Error, SN – observation sample number, R2 – Coefficient of determination).



**Figure 6.** Comparison of phase-specific accuracy metrics Coefficient of determination  $(R^2)$  (a) and *RMSE* (b) for all interpolation results based on filtered and unfiltered phenological observations.



**Figure 7.** JKI data cube environment including the data cubes PHASE, DWD\_TEMP\_MAX, DWD\_Niederschlag and S2\_GermanyGrid.



**Figure 8.** Coupling of data of different geometric and temporal resolution based on a WCS-based query using the example of phenological winter wheat phases (Table 6) and corresponding daily precipitation sums and *SAVI* time series within a parcel.

In the code example 3, the Python function get\_phases\_from\_point is applied to determine the DOYs for the target winter wheat field in 2020. The function is stored in an additional Python file (functions\_DataCube.py). Once the field boundaries are specified (*winterwheat2020.shp*), the function takes six mandatory parameters (target year, crop type, plot centroid coordinates, CRS of the field polygon, and the host address of the data cube) and two optional parameters (to get more information about the WCS request). The function creates a WCS-like URL with the specified parameters and performs the final query using the Python package request. If the query is successful, the function returns the received data in the form of a Python-like list containing all the initial dates of the phenological phases.

In the Jupyter notebook (DemoPhaseWCS.ipynb), we demonstrate how to run this function twice for the target year and the previous year (sowing and emergence of winter wheat), and two other functions for the additional data on the two other data cubes. Both the functions for PHASE data and precipitation data (get\_precipitation\_from\_point) query only a single coordinate due to the coarse spatial resolution of  $1 \times 1 \text{ km}^2$ . In contrast, the function for Sentinel-2 data (get\_tif\_rasdaman) queries an area of interest due to the spatial resolution of  $10 \times 10 \text{ m}^2$ . The received spectral data are then averaged in further *SAVI* processing of the script.

### 243 WCPS-based phase-specific temperature sums

While WCS allows the definition and download of spatio-temporal subsets of the multidimensional data cube (see Data Records section), an OGC-compliant WCPS can be used to integrate the data analysis into a query (see Data Records section). The analysis is performed directly on the data server, where the analysis results are also stored<sup>66</sup>.

Code example 4 shows a WCPS statement for calculating phase-specific temperature totals. The query has been performed for an area near Braunschweig (Germany) for winter wheat phase 18 and the period between 06-10-1999 to 21-05-2000.

<sup>249</sup> The base temperature for winter wheat is 5.5°C. The temperature data is stored with a factor of 10, therefore the sum of

**Code example 3.** Quering PHASE Data Cube using WCS in Python

```
import geopandas as gpd # python package to work with geovector data
1
   from func_DataCube_PHASE import get_phases_from_point # import function from
2
      func_DataCube_PHASE.py
   # directory to shape file of agricultural field'
3
   shp = 'Vector/winterwheat2020.shp'
   # get centroid coodinates from field and transform to CRS: 32632
5
   easting = float(gpd.read_file(shp).to_crs('EPSG:32632').centroid.x)
6
  northing = float(gpd.read_file(shp).to_crs('EPSG:32632').centroid.y)
7
   # get phases from given year
8
   year_on = '2020'
9
   # wcs request:
10
11
   phases_pre = get_phases_from_point(
       year=year_pre, # year
12
       crop='winterwheat', # crop type
13
       easting=easting, # longitude coordinate
14
       northing=northing, # latitude coordinagte
15
       epsg=32632, # crs of input and output
16
       host='https://datacube.julius-kuehn.de/flf/ows', # PHASE Data Cube web adress
17
       printout=False, # if True: information about request process are given
18
       get_query=True) # if True: prints the WCS query URL
19
   print (phases_pre)
20
21
   Output:
22
       https://datacube.julius-kuehn.de/flf/ows?&SERVICE=WCS&VERSION=2.0.1&REQUEST=GetCoverage&
23
           COVERAGEID=PHASE_202_Winterweizen&SUBSET=ansi("2020-01-01")&subsettingCrs=http://ows
           .rasdaman.org/def/crs/EPSG/0/32632&SUBSET=E(595342.5636430825,595342.5636430825)&
           SUBSET=N(5784876.418276947,5784876.418276947)&outputCrs=http://ows.rasdaman.org/def/
           crs/EPSG/0/32632&FORMAT=text/csv
       [106.6466, 144.8433, 175.9788, 192.0013, 206.8396, 281.4659, 292.5806]
24
```

Code example 4. WCPS query

```
for $tMin in (DWD_Temp_Min), $tMax in (DWD_Temp_Max)
   let $t:= [ansi("1999-279":"2000-142")], $p:=[E(3598044), N(5797122)],
2
   $cutout_tmin := $tMin[$t][$p], $cutout_tmax := $tMax[$t][$p]
3
4
   return encode ((condense +
5
       over $d ansi(imageCrsDomain($cutout_tmin, ansi))
6
       using( switch case
7
           (($cutout_tmin[ansi($d)] + $cutout_tmax[ansi($d)]) / 20.0 - 5.5 < 0.0)
8
               return 0.0
9
           default return
10
                ($cutout_tmin[ansi($d)] + $cutout_tmax[ansi($d)]) / 20.0 - 5.5
11
  )) , "csv" )
12
```

PHASE ID	PHASE name	PHASE start	PHASE end	temperature sum
10	Beginning of sowing	1999-279	2000-275	1966.6
12	Emergence	1999-279	1999-292	53.4
15	Beginning of shooting	1999-279	2000-112	267.9
18	Beginning of heading	1999-279	2000-142	574.55
19	Beginning of milk ripening	1999-279	2000-172	885.7
21	Beginning of yellow ripening	1999-279	2000-198	1138.0
24	Harvest	1999-279	2000-218	1363.7

Table 8. Results of WCPS temperature sums queries for a location near Braunschweig and the year 2000 (see code example 4).

the daily maximum temperature and daily minimum temperature must be divided by 20 to obtain the correct average value.

To simplify the query, the day length is left out. The determined temperature sum is 574.55°C. In Table 8, the temperature

sums of the other phases are listed. Note that the growing season of winter crops starts in the year of sowing, here in

<sup>253</sup> 1999. The WCPS statement can also be translated into an URL statement with the following structure https://datacube.julius-

kuehn.de/flf/ows?service=WCS&version=2.0.1&request=ProcessCoverages&query=<WCPS><sup>1</sup>.

## **Code availability**

All **R** functions of the PHASE model are located in the software repository<sup>11</sup> and can be executed by calling the wrapper file

<sup>257</sup> PhaseR.R. In addition, the wrapper file is explained in detail in a corresponding quarto<sup>®</sup> report<sup>67</sup>.

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## **Author contributions statement**

M.M. was the lead author, created the dataset, adapted the PHASE model, documented the model and dataset on Github,

<sup>403</sup> Rpubs and Zenodo, and wrote the original draft. The original model was developed by H.G. who also contributed to the model

description in the manuscript. Supported by P.B., M.D. and P.B. created, curated, described and documented both types of web

<sup>405</sup> services (WCS, WCPS). Together with F.B., M.D. also created an usage note. N.S. described the Bonares Repository. P.H. <sup>406</sup> provided model input data. All authors reviewed the manuscript.

## 407 Competing interests

<sup>408</sup> The authors declare no competing interests.

## 409 Acronyms

- 410 COR Pearson correlation coefficient. 7
- 411 *MAE* Mean Absolute Error. 7, 12
- 412 *MSE* Mean Squared Error. 12
- 413 *RMSE* Root Mean Squared Error. 7, 12, 13
- <sup>414</sup>  $R^2$  Coefficient of determination. 12, 13
- 415 **ARTS** analysis-ready time series. 2, 11
- 416 **DOI** Digital Object Identifier. 2, 10
- 417 **DOY** Day(s) of the Year. 2, 4–7, 9, 11, 14
- <sup>418</sup> **DWD** German Meteorological Service. 1, 2, 5, 6, 11, 12, 19
- 419 **GDD** Growing Degree Days. 2
- 420 GIS geographic information system. 11
- 421 **JKI** Julius Kühn Institute. 12
- 422 **OGC** Open Geospatial Consortium. 11, 14
- **RDM** Research Data Management. 7, 10
- 424 SDI Spatial Data Infrastructure. 7, 10, 12
- 425 VGI volunteered geographical information. 1
- 426 WCPS Web Coverage Processing Service. 11, 12, 14–16
- 427 WCS Web Coverage Service. 2, 11, 12, 14, 15
- 428 **WMS** Web Map Service. 7, 11, 12